Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
S28	14	US-5772874-$.DID. OR US-5795469-$.DID. OR US-5919368-$.DID. OR US-5968367-$.DID. OR US-6107623-$.DID. OR US-6124137-$.DID. OR US-6204500-$.DID. OR US-6268144-$.DID.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 08:12
S29	6	testosteron$5 near5 (mass near2 spectro$7)	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 08:25
S30	6	testosteron$5 near5 ((mass near2 spectro$7) or "mass spectrometry")	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 08:26
S31	2031	testosteron$5 and ((mass near2 spectro$7) or "mass spectrometry")	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 08:26
S32	12	testosteron$5 near10 ((mass near2 spectro$7) or "mass spectrometry")	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 08:30
S33	12	(testosteron$5or testosterone) near10 ((mass near2 spectro$7) or "mass spectrometry")	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 08:54
S34	11	S33 and (quantitat$5 or determinat$5)	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 14:54
S35	6	"l6" and (HTLC or "high turbulence liquid chromatography")	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 14:55
S36	151	(HTLC or "high turbulence liquid chromatography")	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 15:10
S37	15	(HTLC or "high turbulence liquid chromatography") and "mass spectrometry"	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/02/17 15:10

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NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	JAN 26	CA/CAPLUS - Expanded patent coverage to include the Russian Agency for Patents and Trademarks (ROSPATENT)
NEWS	18	FEB 10	STN Patent Forums to be held in March 2005
NEWS	19	FEB 16	STN User Update to be held in conjunction with the 229th ACS National Meeting on March 13, 2005

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

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FILE 'HOME' ENTERED AT 17:10:42 ON 17 FEB 2005

=> file embase biosis medline caplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'EMBASE' ENTERED AT 17:11:02 ON 17 FEB 2005
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=> "mass spectrometry" or "mass spectroscopy"
L1      415056 "MASS SPECTROMETRY" OR "MASS SPECTROSCOPY"

=> MS/MS or TOF
'MS' IS NOT A VALID FIELD CODE
'MS' IS NOT A VALID FIELD CODE
'MS' IS NOT A VALID FIELD CODE
'MS' IS NOT A VALID FIELD CODE
L2       26365 MS/MS OR TOF

=> "MS/MS" or TOF
L3       46722 "MS/MS" OR TOF

=> testosterone and l1
L4        2120 TESTOSTERONE AND L1

=>

=> l3 and l1
L5       31349 L3 AND L1

=> l4 and (quantitation or quantitate or quantification)
L6         190 L4 AND (QUANTITATION OR QUANTITATE OR QUANTIFICATION)

=> l6 and htlc
L7           0 L6 AND HTLC

=> l6 and (turbulence)
L8           0 L6 AND (TURBULENCE)

=> l6 and MALDI
L9           2 L6 AND MALDI

=> d 1-2

L9   ANSWER 1 OF 2  BIOSIS  COPYRIGHT (c) 2005 The Thomson Corporation.  on STN
AN   2003:298564  BIOSIS
DN   PREV200300298564
TI   Derivatisation for the characterisation of neutral oxosteroids by
     electrospray and matrix-assisted laser desorption/ionisation tandem
     mass spectrometry: The Girard P derivative.
AU   Griffiths, William J. [Reprint Author]; Liu, Suya; Alvelius, Gunvor;
     Sjovall, Jan
CS   Department of Medical Biochemistry and Biophysics, Karolinska Institutet,
     SE-17177, Stockholm, Sweden
```

william.griffiths@mbb.ki.se
SO Rapid Communications in Mass Spectrometry, (2003) Vol. 17, No. 9, pp. 924-935. print.
ISSN: 0951-4198 (ISSN print).
DT Article
LA English
ED Entered STN: 25 Jun 2003
Last Updated on STN: 1 Aug 2003

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:367820 CAPLUS
DN 139:142958
TI Derivatisation for the characterisation of neutral oxosteroids by electrospray and matrix-assisted laser desorption/ionisation tandem **mass spectrometry**: The girard P derivative
AU Griffiths, William J.; Liu, Suya; Alvelius, Gunvor; Sjovall, Jan
CS Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Stockholm, SE-17177, Swed.
SO Rapid Communications in Mass Spectrometry (2003), 17(9), 924-935
CODEN: RCMSEF; ISSN: 0951-4198
PB John Wiley & Sons Ltd.
DT Journal
LA English
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> dup rem
ENTER L# LIST OR (END):l9
PROCESSING COMPLETED FOR L9
L10 1 DUP REM L9 (1 DUPLICATE REMOVED)

=> d ibib abs total

L10 ANSWER 1 OF 1 BIOSIS COPYRIGHT (c) 2005 The Thomson Corporation. on STN
DUPLICATE 1
ACCESSION NUMBER: 2003:298564 BIOSIS
DOCUMENT NUMBER: PREV200300298564
TITLE: Derivatisation for the characterisation of neutral oxosteroids by electrospray and matrix-assisted laser desorption/ionisation tandem **mass spectrometry**: The Girard P derivative.
AUTHOR(S): Griffiths, William J. [Reprint Author]; Liu, Suya; Alvelius, Gunvor; Sjovall, Jan
CORPORATE SOURCE: Department of Medical Biochemistry and Biophysics, Karolinska Institutet, SE-17177, Stockholm, Sweden
william.griffiths@mbb.ki.se
SOURCE: Rapid Communications in Mass Spectrometry, (2003) Vol. 17, No. 9, pp. 924-935. print.
ISSN: 0951-4198 (ISSN print).
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 25 Jun 2003
Last Updated on STN: 1 Aug 2003
AB The identification, **quantification** and localization of steroids in biological fluids and tissues are subjects of considerable importance. Not only do steroids have classical hormonal properties via binding to nuclear receptors, they can also elicit cellular responses via interactions with other proteins. For mass spectrometric analysis, neutral steroids are not readily ionized by either electrospray (ES) or matrix-assisted laser desorption/ionization (**MALDI**). In this communication a derivatisation protocol is presented which allows for the rapid analysis of neutral oxosteroids by both ES and **MALDI** **mass spectrometry.** Neutral oxosteroids are derivatised to Girard P hydrazones. When analysed by tandem **mass**

spectrometry the derivatised steroids fragment to give structurally informative spectra allowing subsequent steroid identification. The derivatisation method is simple, the reagents are commercially available, and reaction products are easily isolated from the reaction mixture. Analyte identification can be performed at the sub-pg level.

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=> d his

     (FILE 'HOME' ENTERED AT 17:10:42 ON 17 FEB 2005)

     FILE 'EMBASE, BIOSIS, MEDLINE, CAPLUS' ENTERED AT 17:11:02 ON 17 FEB 2005
L1       415056 "MASS SPECTROMETRY" OR "MASS SPECTROSCOPY"
L2        26365 MS/MS OR TOF
L3        46722 "MS/MS" OR TOF
L4         2120 TESTOSTERONE AND L1
L5        31349 L3 AND L1
L6          190 L4 AND (QUANTITATION OR QUANTITATE OR QUANTIFICATION)
L7            0 L6 AND HTLC
L8            0 L6 AND (TURBULENCE)
L9            2 L6 AND MALDI
L10           1 DUP REM L9 (1 DUPLICATE REMOVED)

=> l5 and (quantitation or quantitate or quantification)
L11       4304 L5 AND (QUANTITATION OR QUANTITATE OR QUANTIFICATION)

=> dup rem l11
PROCESSING IS APPROXIMATELY  65% COMPLETE FOR L11
PROCESSING COMPLETED FOR L11
L12        1680 DUP REM L11 (2624 DUPLICATES REMOVED)

=> l12 and (HTLC or turbulence)
L13           2 L12 AND (HTLC OR TURBULENCE)

=> d l13 1-2

L13  ANSWER 1 OF 2  EMBASE  COPYRIGHT 2005 ELSEVIER INC. ALL RIGHTS RESERVED.
     on STN
AN   1999288241  EMBASE
TI   Comparison of turbulent-flow chromatography with automated solid-phase
     extraction in 96-well plates and liquid-liquid extraction used as plasma
     sample preparation techniques for liquid chromatography-tandem
     mass spectrometry.
AU   Zimmer D.; Pickard V.; Czembor W.; Muller C.
CS   D. Zimmer, Bayer AG, Preclinical Pharmacokinetics, 42096 Wuppertal,
     Germany
SO   Journal of Chromatography A, (1999) 854/1-2 (23-35).
     Refs: 6
     ISSN: 0021-9673  CODEN: JCRAEY
PUI  S 0021-9673(99)00535-X
CY   Netherlands
DT   Journal; Conference Article
FS   029     Clinical Biochemistry
     030     Pharmacology
LA   English
SL   English

L13  ANSWER 2 OF 2  BIOSIS  COPYRIGHT (c) 2005 The Thomson Corporation.  on STN
AN   2000:132714  BIOSIS
DN   PREV200000132714
TI   Quantitative analysis of terbinafine (Lamisil(R)) in human and minipig
     plasma by liquid chromatography tandem mass spectrometry
AU   Brignol, N.; Bakhtiar, R. [Reprint author]; Dou, L.; Majumdar, T.; Tse, F.
```

L. S.
CS Novartis, 59 Route 10, Building 405, Room 229, East Hanover, NJ, 07936, USA
SO Rapid Communications in Mass Spectrometry, (2000) Vol. 14, No. 3, pp. 141-149. print.
CODEN: RCMSEF. ISSN: 0951-4198.
DT Article
LA English
ED Entered STN: 12 Apr 2000
Last Updated on STN: 4 Jan 2002

=> d ibib abs total

L13 ANSWER 1 OF 2 EMBASE COPYRIGHT 2005 ELSEVIER INC. ALL RIGHTS RESERVED. on STN
ACCESSION NUMBER: 1999288241 EMBASE
TITLE: Comparison of turbulent-flow chromatography with automated solid-phase extraction in 96-well plates and liquid-liquid extraction used as plasma sample preparation techniques for liquid chromatography-tandem **mass spectrometry.**
AUTHOR: Zimmer D.; Pickard V.; Czembor W.; Muller C.
CORPORATE SOURCE: D. Zimmer, Bayer AG, Preclinical Pharmacokinetics, 42096 Wuppertal, Germany
SOURCE: Journal of Chromatography A, (1999) 854/1-2 (23-35). Refs: 6
ISSN: 0021-9673 CODEN: JCRAEY
PUBLISHER IDENT.: S 0021-9673(99)00535-X
COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Conference Article
FILE SEGMENT: 029 Clinical Biochemistry
030 Pharmacology
LANGUAGE: English
SUMMARY LANGUAGE: English
AB Turbulent flow chromatography (TFC) combined with the high selectivity and sensitivity of tandem **mass spectrometry** (**MS-MS**) is a new technique for the fast direct analysis of drugs from crude plasma. TFC in the 96-well plate format reduces significantly the time required for sample clean-up in the laboratory. For example, for 100 samples the workload for a technician is reduced from about 8 h by a manual liquid-liquid extraction (LLE) assay to about 1 h in the case of TFC. Sample clean-up and analysis are performed on-line on the same column. Similar chromatographic performance and validation results were achieved using **HTLC** Turbo-C18 columns (Cohesive Technologies) and Oasis HLB extraction columns (Waters). One 96-well plate with 96 plasma samples is analyzed within 5.25 h, corresponding to 3.3 min per sample. Compared to this LLE and analysis of 96 samples takes about 16 h. Two structurally different and highly protein bound compounds, drug A and drug B, were analyzed under identical TFC conditions and the assays were fully validated for the application to toxicokinetics studies (compliant with Good Laboratory Practices - GLP). The limit of **quantitation** was 1.00 μg/l and the linear working range covered three orders of magnitude for both drugs. In the case of drug A the quality of analysis by TFC was similar to the reference LLE assay and slightly better than automated solid-phase extraction in 96-well plates. The accuracy was -3.1 to 6.7% and the precision was 3.1 to 6.8% in the case of drug A determined for dog plasma by TFC-**MS-MS.** For drug B the accuracy was -3.7 to 3.5% and the precision was 1.6 to 5.4% for rat plasma, which is even slightly better than what was achieved with the validated protein precipitation assay. Copyright (C) 1999 Elsevier Science B.V.

L13 ANSWER 2 OF 2 BIOSIS COPYRIGHT (c) 2005 The Thomson Corporation. on STN
ACCESSION NUMBER: 2000:132714 BIOSIS
DOCUMENT NUMBER: PREV200000132714

TITLE: Quantitative analysis of terbinafine (Lamisil(R)) in human and minipig plasma by liquid chromatography tandem **mass spectrometry.**
AUTHOR(S): Brignol, N.; Bakhtiar, R. [Reprint author]; Dou, L.; Majumdar, T.; Tse, F. L. S.
CORPORATE SOURCE: Novartis, 59 Route 10, Building 405, Room 229, East Hanover, NJ, 07936, USA
SOURCE: Rapid Communications in Mass Spectrometry, (2000) Vol. 14, No. 3, pp. 141-149. print.
CODEN: RCMSEF. ISSN: 0951-4198.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 12 Apr 2000
Last Updated on STN: 4 Jan 2002

AB A method using liquid chromatography/tandem **mass spectrometry** (LC/**MS/MS**) for the determination of terbinafine in human and minipig plasma has been developed and validated. The method used positive-ion mode for monitoring terbinafine, and used a stable isotope labelled terbinafine as the internal standard. Subsequent to acetonitrile protein precipitation, the supernatant was directly (unfiltered) injected onto the LC column (retention time apprx4.3 min) for analysis. Interday and intraday accuracy and precision were assessed from the relative recoveries (observed concentration in percent of the nominal value) of spiked samples analyzed on three different days. The lower limit of **quantitation** (LLOQ) was 0.0679 ng/mL in human and minipig using a plasma sample volume of 0.08 mL. The method was fast, specific, and exhibited ruggedness. Furthermore, the use of turbulent flow chromatography (TurboFlow LC/**MS/MS**) coupled to **mass spectrometry** for direct analysis of terbinafine in plasma is discussed. The technique allowed direct introduction of plasma with satisfactory chromatographic peak shape and increased throughput.

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=> d his

     (FILE 'HOME' ENTERED AT 17:10:42 ON 17 FEB 2005)

     FILE 'EMBASE, BIOSIS, MEDLINE, CAPLUS' ENTERED AT 17:11:02 ON 17 FEB 2005
L1       415056 "MASS SPECTROMETRY" OR "MASS SPECTROSCOPY"
L2        26365 MS/MS OR TOF
L3        46722 "MS/MS" OR TOF
L4         2120 TESTOSTERONE AND L1
L5        31349 L3 AND L1
L6          190 L4 AND (QUANTITATION OR QUANTITATE OR QUANTIFICATION)
L7            0 L6 AND HTLC
L8            0 L6 AND (TURBULENCE)
L9            2 L6 AND MALDI
L10           1 DUP REM L9 (1 DUPLICATE REMOVED)
L11        4304 L5 AND (QUANTITATION OR QUANTITATE OR QUANTIFICATION)
L12        1680 DUP REM L11 (2624 DUPLICATES REMOVED)
L13           2 L12 AND (HTLC OR TURBULENCE)

=> (l4 or l6) and nitrogen
L14          25 (L4 OR L6) AND NITROGEN

=> d scan

L14   25 ANSWERS   CAPLUS  COPYRIGHT 2005 ACS on STN
CC    80-4 (Organic Analytical Chemistry)
      Section cross-reference(s): 17, 51, 64
TI    Fast, high temperature and thermolabile GC-MS in supersonic molecular
      beams
ST    fast thermolabile GCMS supersonic mol beam; high temp GCMS supersonic mol
      beam; gasoline analysis GCMS supersonic mol beam; pharmaceutical analysis
      GCMS supersonic mol beam; food analysis GCMS supersonic mol beam;
```

ethyllead detn GCMS supersonic mol beam; caffeine detn GCMS supersonic mol beam; codeine detn GCMS supersonic mol beam

IT Amino acids, analysis
Steroids, analysis
RL: ANT (Analyte); ANST (Analytical study)
(anal. of, by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT Coffee (Coffea)
(caffeine determination in, by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT Aromatic compounds
RL: ANT (Analyte); ANST (Analytical study)
(detection of, by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT Pharmaceutical analysis
(fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam for)

IT Gasoline
RL: AMX (Analytical matrix); ANST (Analytical study)
(lead and aromatic determination in, by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT Aromatic hydrocarbons, analysis
RL: ANT (Analyte); ANST (Analytical study)
(halo, detection of, by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT Chromatography, gas
(high-temperature, supersonic mol. beam **mass spectrometry** combined with fast, for anal.)

IT **Mass spectrometry**
(mol.-beam, fast and high-temperature and thermolabile gas chromatog. combined with supersonic, for anal.)

IT Heterocyclic compounds
RL: ANT (Analyte); ANST (Analytical study)
(**nitrogen**, anal. of, by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT Aromatic hydrocarbons, analysis
RL: ANT (Analyte); ANST (Analytical study)
(polycyclic, detection of, by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT Volatile substances
(semi-, detection of, by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT Molecular beams
(supersonic, in fast and high-temperature and thermolabile gas chromatog./**mass spectrometry**)

IT 1719-06-8, Anthracene-d10 74232-90-9, Anthracene-d9 159510-21-1, Anthracene-d8
RL: ANT (Analyte); ANST (Analytical study)
(determination of, by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT 58-08-2, Caffeine, analysis
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in coffee by fast and high-temperature and thermolabile gas chromatog./**mass spectrometry** in supersonic mol. beam)

IT 76-57-3, Codeine
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in drugs by fast and high-temperature and thermolabile gas
chromatog./**mass spectrometry** in supersonic mol. beam)
IT 78-00-2, Tetraethyllead
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in gasoline by fast and high-temperature and thermolabile gas
chromatog./**mass spectrometry** in supersonic mol. beam)
IT 54-11-5, Nicotine 57-83-0, Pregn-4-ene-3,20-dione, analysis 57-88-5, Cholest-5-en-3-ol (3β)-, analysis 58-22-0, **Testosterone** 63-91-2, L-Phenylalanine, analysis 71-43-2, Benzene, analysis 108-86-1, Bromobenzene, analysis 108-90-7, Chlorobenzene, analysis 112-61-8, Methyl stearate 120-73-0, Purine 147-85-3, L-Proline, analysis 190-26-1, Ovalene 191-07-1, Coronene 198-55-0, Perylene 574-93-6, Phthalocyanine 591-50-4, Iodobenzene 1912-24-9, Atrazine
RL: ANST (Analytical study)
(fast and high-temperature and thermolabile gas chromatog./supersonic mol. beam **mass spectrometry** of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L14 25 ANSWERS BIOSIS COPYRIGHT (c) 2005 The Thomson Corporation. on STN
TI Identification of the aromatase inhibitor aminoglutethimide in urine by gas chromatography/**mass spectrometry.**
IT Methods & Equipment
gas chromatography: chromatographic techniques, laboratory techniques; **mass spectrometry**: laboratory techniques, spectrum analysis techniques

L14 25 ANSWERS CAPLUS COPYRIGHT 2005 ACS on STN
CC 64-1 (Pharmaceutical Analysis)
TI A new capillary-scale liquid chromatography-**mass spectrometry** interface for the generation of electron ionization spectra
ST drug analysis liq chromatog mass spectrometr
IT Liquid chromatography
Mass spectrometry
Pharmaceutical analysis
(drug anal. by capillary-scale liquid chromatog.-**mass spectrometry** interface for generation of electron ionization spectra)
IT 58-22-0, **Testosterone** 99-50-3, 3,4-Dihydroxybenzoic acid 43121-43-3, Triadimefon
RL: ANT (Analyte); ANST (Analytical study)
(drug anal. by capillary-scale liquid chromatog.-**mass spectrometry** interface for generation of electron ionization spectra)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d his

(FILE 'HOME' ENTERED AT 17:10:42 ON 17 FEB 2005)

FILE 'EMBASE, BIOSIS, MEDLINE, CAPLUS' ENTERED AT 17:11:02 ON 17 FEB 2005
L1 415056 "MASS SPECTROMETRY" OR "MASS SPECTROSCOPY"
L2 26365 MS/MS OR TOF
L3 46722 "MS/MS" OR TOF
L4 2120 TESTOSTERONE AND L1
L5 31349 L3 AND L1
L6 190 L4 AND (QUANTITATION OR QUANTITATE OR QUANTIFICATION)

```
L7             0 L6 AND HTLC
L8             0 L6 AND (TURBULENCE)
L9             2 L6 AND MALDI
L10            1 DUP REM L9 (1 DUPLICATE REMOVED)
L11         4304 L5 AND (QUANTITATION OR QUANTITATE OR QUANTIFICATION)
L12         1680 DUP REM L11 (2624 DUPLICATES REMOVED)
L13            2 L12 AND (HTLC OR TURBULENCE)
L14           25 (L4 OR L6) AND NITROGEN

=> l14 and (CID or "collision induced dissociation")
L15            0 L14 AND (CID OR "COLLISION INDUCED DISSOCIATION")

=> l14 and (CID)
L16            0 L14 AND (CID)

=> (l4 or l6) and CID
L17           13 (L4 OR L6) AND CID

=> l17 and nitrogen
L18            0 L17 AND NITROGEN

=> d his

     (FILE 'HOME' ENTERED AT 17:10:42 ON 17 FEB 2005)

     FILE 'EMBASE, BIOSIS, MEDLINE, CAPLUS' ENTERED AT 17:11:02 ON 17 FEB 2005
L1         415056 "MASS SPECTROMETRY" OR "MASS SPECTROSCOPY"
L2          26365 MS/MS OR TOF
L3          46722 "MS/MS" OR TOF
L4           2120 TESTOSTERONE AND L1
L5          31349 L3 AND L1
L6            190 L4 AND (QUANTITATION OR QUANTITATE OR QUANTIFICATION)
L7              0 L6 AND HTLC
L8              0 L6 AND (TURBULENCE)
L9              2 L6 AND MALDI
L10             1 DUP REM L9 (1 DUPLICATE REMOVED)
L11          4304 L5 AND (QUANTITATION OR QUANTITATE OR QUANTIFICATION)
L12          1680 DUP REM L11 (2624 DUPLICATES REMOVED)
L13             2 L12 AND (HTLC OR TURBULENCE)
L14            25 (L4 OR L6) AND NITROGEN
L15             0 L14 AND (CID OR "COLLISION INDUCED DISSOCIATION")
L16             0 L14 AND (CID)
L17            13 (L4 OR L6) AND CID
L18             0 L17 AND NITROGEN

=> dup rem l17
PROCESSING COMPLETED FOR L17
L19             7 DUP REM L17 (6 DUPLICATES REMOVED)

=> d ibib abs total

L19  ANSWER 1 OF 7     MEDLINE on STN                    DUPLICATE 1
ACCESSION NUMBER:   2005068643     IN-PROCESS
DOCUMENT NUMBER:    PubMed ID: 15700167
TITLE:              Application of pentafluorophenyl hydrazine derivatives to
                    the analysis of nabumetone and testosterone in
                    human plasma by liquid chromatography-atmospheric pressure
                    chemical ionization-tandem mass
                    spectrometry.
AUTHOR:             Sheen J F; Her G R
CORPORATE SOURCE:   Department of Chemistry, National Taiwan University,
                    Taipei, Taiwan.. grher@mail.ch.ntu.edu.tw
SOURCE:             Analytical and bioanalytical chemistry, (2004 Dec) 380
                    (7-8) 891-7.
                    Journal code: 101134327. ISSN: 1618-2642.
```

PUB. COUNTRY: Germany: Germany, Federal Republic of
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: IN-PROCESS; NONINDEXED; Priority Journals
ENTRY DATE: Entered STN: 20050209
Last Updated on STN: 20050211

AB Two carbonyl compounds, nabumetone and **testosterone**, were derivatized with pentafluorophenyl hydrazine (PFPH) and analyzed by atmospheric-pressure chemical-ionization **mass spectrometry**. The PFPH derivatives underwent dissociative electron capture in negative-ion APCI (ECAPCI) and gave intense [M-20](-) ions in the mass spectra. In positive-ion APCI, the PFPH derivatives underwent efficient protonation and gave intense [M + H](+) ions in the mass spectra. In **CID**, the major product ions of the [M-20](-) ions in ECAPCI corresponded to the partial moiety of PFPH. In contrast, the major product ions of [M + H](+) corresponded to the partial moiety of the analyte. By using selected reaction monitoring (SRM) detection, low pg of nabumetone (1 pg) and **testosterone** (7 pg) could be detected in both ECAPCI and positive-ion APCI. In comparison with the detection limits (SRM) of the underivatized analytes, use of the PFPH derivatives resulted in 2500-fold and 35-fold sensitivity enhancements for nabumetone and **testosterone**, respectively. The PFPH derivatives were applied to the analysis of nabumetone and **testosterone** in human plasma by both ECAPCI and positive-ion APCI and were found to enable detection of 0.1 ng mL(-1) nabumetone in spiked plasma. For **testosterone**, endogenous **testosterone** in female plasma was detected in both ECAPCI and positive-ion APCI.

L19 ANSWER 2 OF 7 MEDLINE on STN
ACCESSION NUMBER: 2004158810 MEDLINE
DOCUMENT NUMBER: PubMed ID: 15052556
TITLE: Creation and comparison of MS/MS spectral libraries using quadrupole ion trap and triple-quadrupole mass spectrometers.
AUTHOR: Josephs Jonathan L; Sanders Mark
CORPORATE SOURCE: Bristol-Myers Squibb, Pharmaceutical Research Institute, New Brunswick, NJ 08543-5400, USA.. jonathan.josephs@bms.com
SOURCE: Rapid communications in mass spectrometry : RCM, (2004) 18 (7) 743-59.
Journal code: 8802365. ISSN: 0951-4198.
PUB. COUNTRY: England: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200407
ENTRY DATE: Entered STN: 20040331
Last Updated on STN: 20040722
Entered Medline: 20040721

AB Searchable libraries of MS/MS spectra, obtained using liquid chromatography/tandem **mass spectrometry** (LC/MS/MS) with data-dependent scan mode switching on both quadrupole ion trap and triple-quadrupole mass spectrometers in conjunction with electrospray ionization, are presented. The effects on library search scores of changing the parameters for producing collision-induced dissociation (**CID**) on both instrument types are systematically evaluated. These observations serve as a basis for determining a universal set of conditions for building MS/MS libraries. A group of 19 closely related steroids was used. The ability to obtain library-searchable spectra at low concentrations is demonstrated for the analysis of a sample of progesterone spiked with hydroxyprogesterone impurities at 0.1 and 0.01%.

L19 ANSWER 3 OF 7 BIOSIS on STN
DUPLICATE 2

ACCESSION NUMBER: 2001:427049 BIOSIS
DOCUMENT NUMBER: PREV200100427049
TITLE: Liquid chromatography tandem **mass spectrometry** applied to the analysis of natural and synthetic steroids in environmental waters.
AUTHOR(S): Lagana, A. [Reprint author]; Fago, G.; Marino, A.; Santarelli, D.
CORPORATE SOURCE: Department of Chemistry, "La Sapienza" University, P.le Aldo Moro 5, 00185, Roma, Italy
aldo.lagana@uniroma1.it
SOURCE: Analytical Letters, (April, 2001) Vol. 34, No. 6, pp. 913-926. print.
CODEN: ANALBP. ISSN: 0003-2719.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 12 Sep 2001
Last Updated on STN: 22 Feb 2002

AB A multiresidue analytical method for the determination of the most common and biologically active natural and synthetic steroids (four estrogens: estriol, 17beta-estradiol, 17alpha-ethynylestradiol, estrone; one progestagen: progesterone and six androgens: trenbolone, boldenone, nandrolone, **testosterone**, 17alpha-methyltestosterone, stanozolol) in environmental waters was developed. The analytes were isolated from water samples by solid phase extraction (SPE) utilizing a graphitized carbon black adsorbent (Carbograph-1). The final samples were analyzed by reversed-phase high performance liquid chromatography with tandem **mass spectrometry** using atmospheric pressure chemical ionization (LC-APCI-MS-MS). Ionization was performed in a heated nebulizer (HN) interface operating in the positive ion mode. The protonated ions (M+H)+ and the dehydrated ions (M+H-H2O)+ (for estriol, 17alpha-estradiol, 17beta-estradiol, and 17alpha-ethynylestradiol) were used as precursor ion for collision-induced dissociation (**CID**), and two diagnostic product ions for each analyte were identified for the unambiguous steroid confirmation by multiple reaction monitoring (MRM) mode. Method performance, for this analytical procedure, was validated by analyzing groundwater and river water samples fortified at level of 20 ng/L. The average recovery for each analyte exceeded 82%. Good method precision was demonstrated with percent relative standard deviation of less than 7.2% for all analytes.

L19 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:211269 CAPLUS
DOCUMENT NUMBER: 132:330020
TITLE: Analysis of oxosteroids by nano-electrospray **mass spectrometry** of their oximes
AUTHOR(S): Liu, Suya; Sjovall, Jan; Griffiths, William J.
CORPORATE SOURCE: Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Stockholm, SE-171 77, Swed.
SOURCE: Rapid Communications in Mass Spectrometry (2000), 14(6), 390-400
CODEN: RCMSEF; ISSN: 0951-4198
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A method for the anal. of neutral oxosteroids by electrospray **mass spectrometry** is described. The oxosteroids are converted into their oximes by treatment with hydroxyammonium chloride in aqueous methanol. Intense peaks corresponding to protonated oxime mols. are observed in nano-electrospray mass spectra. The detection limits for the oximes of progesterone, pregnenolone and dehydroepiandrosterone were 2.5, 5 and 25 pg/μL, resp., approx. 20 times lower than for the underivatized steroids. The signal intensities were proportional to the concentration of the steroids in the range of 500 to 2.5 pg/μL. Fragmentation by collision-induced dissociation (**CID**) was studied using oximes of 28 model steroids carrying an oxo group at C-3, C-17 or C-20. Some of the

steroid oximes were labeled with deuterium or 15N. Fragment ions were observed which yielded useful structural information. Upon **CID**, protonated oximes of 3-oxo-Δ4-steroids produced abundant ions by cleavage through the B-ring and by loss of the side chain, while protonated oximes of saturated 3-oxosteroids did not give abundant ions by cleavage through the B-ring. Protonated oximes of 20-oxosteroids unsubstituted at C-21, C-17 or C-16 produced a characteristic ion at m/z 86 containing the side chain, C-16 and C-17. Protonated oximes of steroids containing only a 17-oxo group gave fewer ions of diagnostic value. Coupled with the selective isolation of steroid oximes from a biol. matrix this method of derivatization and **CID** may be used for the anal. of neutral oxosteroids in biol. samples.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 7 EMBASE COPYRIGHT 2005 ELSEVIER INC. ALL RIGHTS RESERVED. on STN DUPLICATE 3

ACCESSION NUMBER: 1999118647 EMBASE

TITLE: Electrospray collision-induced dissociation of **testosterone** and **testosterone** hydroxy analogs.

AUTHOR: Williams T.M.; Kind A.J.; Houghton E.; Hill D.W.

CORPORATE SOURCE: D.W. Hill, Microchemistry Laboratory, U-193, University of Connecticut, 3113 Horsebarn Road, Storrs, CT 06269, United States. hill@uconnvm.uconn.edu

SOURCE: Journal of Mass Spectrometry, (1999) 34/3 (206-216). Refs: 16
ISSN: 1076-5174 CODEN: JMSPFJ

COUNTRY: United Kingdom

DOCUMENT TYPE: Journal; Article

FILE SEGMENT: 029 Clinical Biochemistry

LANGUAGE: English

SUMMARY LANGUAGE: English

AB Complications with the gas chromatographic analysis of steroids prompted the use of alternative techniques for their identification. High-performance liquid chromatography/**mass spectrometry** with atmospheric pressure ionization allowed the collection of data for structural identification of these compounds. The objective of this study was to investigate the up-front collision-induced dissociation (UFCID) electrospray ionization (ESI) mass spectra of **testosterone** and monohydroxylated **testosterones**. The positive ion UFCID ESI mass spectrum of **testosterone** showed three significant ions at m/z 97, 109 and 123. The relative abundance of these ions in the UFCID ESI mass spectra of monohydroxylated **testosterones** varied with the position of the hydroxy group. Statistical data allowed the prediction of hydroxy group position on **testosterone** by evaluation of the relative abundance of the m/z 97, 109, 121 and 123 ions. Data from the ESI mass spectral analysis of **testosterone** in a deuterated solvent and from the analysis of cholestenone and 4-androstene-3β,17β-diol indicated that the initial ionization of **testosterone** occurred at the 3-one position. **CID** parent ion monitoring analyses of the m/z 97, 109 and 123 ions indicated that each resulted from different fragmentation mechanisms and originated directly from the [M+H]+ parent ion. The elemental composition of these fragment ions is proposed based on evidence gathered from the **CID** analysis of the pseudo-molecular ions of [1,2-2H2]-, [2,2,4,6,6-2H5]-, [6,7-2H]-, [7-2H]-, [19,19,19-2H3]- and [3,4-13C2]**testosterone**. The structure and a possible mechanism of formation of the m/z 109 and 123 ions is presented. The results of this study advance the understanding of the mechanisms of collision-induced fragmentation of ions.

L19 ANSWER 6 OF 7 BIOSIS COPYRIGHT (c) 2005 The Thomson Corporation. on STN DUPLICATE 4

ACCESSION NUMBER: 1997:405337 BIOSIS

DOCUMENT NUMBER: PREV199799711540

TITLE: Confirmation of anabolic hormone residues in bovine blood by micro-HPLC-ion spray-tandem **mass spectrometry.**

AUTHOR(S): Draisci, Rosa [Reprint author]; Giannetti, Luigi; Lucentini, Luca; Purificato, Luca Vv Palleschiana; Moretti, Gabriella

CORPORATE SOURCE: Lab. di Med. Veterinaria, Ist. Superiore di Sanita, v.le Regina Elena 299, 00161 Roma, Italy

SOURCE: HRC Journal of High Resolution Chromatography, (1997) Vol. 20, No. 8, pp. 421-430.
CODEN: JHRCE7. ISSN: 0935-6304.

DOCUMENT TYPE: Article

LANGUAGE: English

ENTRY DATE: Entered STN: 24 Sep 1997
Last Updated on STN: 21 Nov 1997

AB Sensitive, specific analytical methods for the determination of anabolics in biological matrices are essential to control the illegal use of these substances in food-producing animals. Programs of residue control are performed annually in Italy for the determination of endogenous sex hormones (17-beta-estradiol, progesterone, **testosterone**) for which maximum physiological levels have been established. At present, the methods used in the Italian programs to determine natural hormones in bovine blood are based on the sensitive radioimmunoassay (RIA), due to relatively low levels of these substances in plasma/serum. In this study, we report a new method based on tandem **mass spectrometry** with on-line micro-high performance liquid chromatography (micro-HPLC-MS-MS) using an atmospheric pressure ionization (API) source and an ion spray (IS) interface for the specific direct detection of natural (progesterone and **testosterone**), and synthetic (17-beta-19-nortestosterone and medroxyprogesterone) hormone residues in bovine serum. 17-Methyltestosterone was used as the internal standard. Analytes were extracted with acetate buffer, purified on C18 Solid Phase Extraction (SPE) cartridge and separated on a reverse phase C18 microHPLC column (300 mm times 1 mm, 5 gm), using acetonitrile-water, 80:20 (v/v) containing 2 mM ammonium acetate as the mobile phase, at a flow rate of 10 mu-l/min. When anabolic hormones were ionized in the IS interface operating in the positive ion mode, only the protonated molecules, (M+H)+, were generated, without evidence of any fragmentation. These served as precursor ions for collision induced dissociation (**CID**) and diagnostic daughter ions for each analyte were identified in order to carry out analysis by microHPLC-MS-MS in the selected reaction monitoring (SRM) mode. For the analytes in question, the response of the mass detector was related linearly to the quantity of each analyte injected between 10 and 300 pg, in the SRM mode. The limit of detection, based on a 3:1 signal-to-noise ratio, is 6-7 pg for the hormones. Recoveries were higher than 83% for 17-beta-19-nortestosterone, **testosterone**, and 17-methyltestosterone, and 72% for medroxyprogesterone, and progesterone. The micro-HPLC-MS-MS method for the determination of anabolic hormones in bovine blood requires no sample derivatization, minimal sample preparation, and provides a sensitive, selective, rapid alternative to the existing purification, separation, and detection techniques. At present this very sensitive method is being successfully applied to measure bovine serum concentrations of natural hormones, such as **testosterone** and progesterone, in order to then confirm any illegal administration of these substances.

L19 ANSWER 7 OF 7 MEDLINE on STN

ACCESSION NUMBER: 96290812 MEDLINE

DOCUMENT NUMBER: PubMed ID: 8728507

TITLE: Identification of the heme adduct and an active site peptide modified during mechanism-based inactivation of rat liver cytochrome P450 2B1 by secobarbital.

AUTHOR: He K; Falick A M; Chen B; Nilsson F; Correia M A

CORPORATE SOURCE: Department of Cellular and Molecular Pharmacology, University of California, San Francisco 94143, USA.

CONTRACT NUMBER: DK 26506 (NIDDK)
NIADKK 26743 (ADAMHA)
RR-01614 (NCRR)
SOURCE: Chemical research in toxicology, (1996 Apr-May) 9 (3) 614-22.
Journal code: 8807448. ISSN: 0893-228X.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199610
ENTRY DATE: Entered STN: 19961022
Last Updated on STN: 19961022
Entered Medline: 19961010

AB The olefinic barbiturate secobarbital (SB) is a sedative hypnotic known to be a relatively selective mechanism-based inactivator of rat liver cytochrome P450 2B1. Previous studies have demonstrated that such inactivation results in prosthetic heme destruction and irreversible drug-induced protein modification, events most likely triggered by P450 2B1-dependent oxidative activation of the olefinic pi-bond. However, the precise structure of the SB-modified heme and/or the protein site targeted for attack remained to be elucidated. We have now isolated the SB-heme adduct from P450 2B1 inactivated by [14C]SB in a functionally reconstituted system and structurally characterized it by electronic absorption spectroscopy and tandem collision-induced dissociation (**CID**), matrix-assisted laser desorption ionization on time of flight (MALDI-TOF), and liquid secondary ion **mass spectrometry** in the positive mode (+ LSIMS) as the N-(5-(2-hydroxypropyl)-5-(1-methylbutyl)barbituric acid)protoporphyrin IX adduct. The [14C]SB-modified 2B1 protein has also been isolated from similar inactivation systems and subjected to lysyl endopeptidase C (Lys-C) digestion and HPLC-peptide mapping. A [14C]SB-modified 2B1 peptide was thus isolated, purified, electrotransferred onto a poly-(vinylidene) membrane, and identified by micro Edman degradation of its first N-terminal 17 residues (S277NH(H)TEFH(H)ENLMISLL293) as the Lys-C peptide domain comprised of amino acids 277-323. This peptide thus includes the peptide domain corresponding to the distal helix I of P450 101, a region highly conserved through evolution, and which is known not only to flank the heme moiety but also to intimately contact the substrates. This finding thus suggests that SB-induced protein modification of P450 2B1 also occurs at the active site and, together with heme N-alkylation, contributes to the SB-induced mechanism-based inactivation of P450 2B1.